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TECHNICAL REPORT #6

LOW-ENERGY ELECTRON DIFFRACTION STUDY OF THE SURFACE-
DEFECT STRUCTURE OF Ge GROWN EPITAXIALLY ON GaAs(110)

by

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Defects in the geometrical structure of a surface can have significant impact on the electronic and chemical properties of a material. A correlation of structural defects with changes in the electronic and chemical properties is therefore important in many technologies (e.g., semiconductor device fabrication, catalysis, and corrosion). A first step in such a correlation is to characterize quantitatively the defect structure of surfaces. This abstract summarizes initial results of an investigation of the surface defects in Ge films grown epitaxially on cleaved GaAs(110).

The Ge/GaAs interface has in recent years received considerable attention. Most of the effort has centered on characterizing the electronic properties of the interface, i.e., band gap discontinuities⁽¹⁻⁴⁾, localized bonding^(3,5), work function changes⁽⁵⁾ and abruptness⁽³⁻⁵⁾ of the interface. X-ray and ultraviolet photoelectron spectroscopy have been used as the main analytical techniques in these investigations. Structural studies of the Ge/GaAs interface are quite limited^(5,6). We are not aware of any attempts to determine the influence of surface defects on the electronic properties of the Ge/GaAs interface.

Because of the small lattice mismatch involved, it is possible to grow nearly strain-free films of Ge on GaAs. Hence, Ge grown epitaxially on GaAs is an important model system for studying the effects of substrate order and deposition parameters on film growth. We have analyzed the angular profiles of diffracted beams in low-energy electron diffraction (LEED) patterns obtained from epitaxial Ge overlayers. Defects such as mosaic structure, strain, and finite-island size,⁽⁷⁾ as well as steps⁽⁸⁾ can at present be quantitatively studied by making this type of measurement. We have chosen initially to grow thick ($>100\text{\AA}$) Ge overlayers. By growing thick layers, one can in principle separate those substrate defects that

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may have longer-range influence on the structural quality of the epitaxial film from those that do not.

The apparatus has been described in detail elsewhere.⁽⁹⁾ A vidicon camera is used to record the intensity distribution in the LEED pattern displayed on a fluorescent screen. The vidicon is aligned so that it scans along a particular azimuth of the LEED pattern. The intensity along that azimuth is digitized and is transferred to an on-line computer for storage and subsequent analysis. The recorded angular profile thus represents the intensity distribution in θ , the exit angle as measured from the surface normal. Ge was deposited onto cleaved GaAs(110) substrates at a rate of $\sim 4 \text{ \AA/minute}$, as measured by a quartz crystal thickness monitor placed at the sample position. High-purity Ge was evaporated at an ambient pressure of 1×10^{-8} torr, measured with a partial pressure analyzer. Background gases during deposition were those typically observed in UHV systems. Initial depositions were performed on undoped GaAs substrates that were heated to 350 and 450°C. Substrate temperatures T_s of 450 and 540°C were used for later depositions on Cr-doped, semi-insulating GaAs. Auger electron spectroscopy was used to check for contamination in the Ge film and on the GaAs substrate. Annealing caused increased interdiffusion of Ga and As into Ge, as measured by AES depth profiling, with As observable on the Ge surface.

Before each Ge deposition, the defect structure of the cleaved GaAs(110) surface was investigated. This involved measuring the angular profiles of the diffracted beam (I vs θ) as a function of primary electron energy. Any broadening of the diffracted beams beyond that contributed by the instrument is due to defects. We interpret the LEED beam broadening, $\delta\theta$, in terms of the parallel and perpendicular components of the momentum transfer vector (i.e. $S_{||}$ and S_{\perp}). By studying the changes in $S_{||}$ and S_{\perp} as a function of

energy and order of diffracted beams, it is possible to separate the effects of strain, mosaic structure, finite-size domains, and steps.⁽⁷⁾ Identical measurements were made on the as-deposited Ge layer. The layer was then annealed for 30 minutes at 600°C and the angular profile measurements were repeated.

The substrates all produced sharp (1x1) LEED patterns that exhibited very little background intensity at all energies. At certain energies, the angular widths of the diffracted beams appear to be instrument-limited (within the error of the experiment)--indicative of very large domains. At other energies, however, the beams show a definite broadening beyond that due to the instrument response. The width of the (01) beam does not exhibit the oscillatory dependence on energy that is characteristic of a surface that has a finite concentration of monatomic steps.⁽⁸⁾ If the broadening is interpreted in terms of finite domain size and finite misorientations, an average domain size of $1200 \pm 600 \text{ \AA}$ and an average out-of-plane misorientation of $\pm 0.12^\circ$ is obtained. The error is large because the widths of the diffracted beams are not broadened appreciably beyond the instrument response function.

The 1200 \AA domain size that we have obtained for the substrates by interpreting the broadening in terms of mosaic structure and monatomic steps represents a lower limit to the actual domain size. We have not considered, in this interpretation, the possible existence of multiautomic steps. These multiautomic steps may be generated during the cleavage process when planes of atoms slip into equivalent lattice sites. Because the slip is by an integral multiple of the bulk interlayer distance, slip planes act like coherent steps of varying heights. Assuming that

these "steps" have random heights, the simple, oscillatory energy dependence of the diffracted beam widths will not be observed. Although diffracted beams will still be sharp at the energies corresponding to minima for monatomic steps, the maxima between them will be washed out. If we make the simplistic assumption that all of the slip planes are the same height, so that Henzler's model for monatomic steps⁽⁸⁾ can be applied, we obtain a maximum slip plane concentration of 2%. This corresponds to an average terrace width of 280\AA for GaAs(110).

The LEED patterns obtained from the as-grown Ge overlayers were qualitatively poorer than those obtained from the corresponding substrates. They also contained fewer spots than the substrate LEED patterns, as expected. Superlattices⁽⁵⁾ were not observed. A film grown at $T_s = 450^\circ\text{C}$ and annealed at 600°C for a short time yielded⁽¹⁰⁾ a domain size of 55\AA , and an average misorientation of $\pm 0.12^\circ$. The behavior of overlayers grown at $T_s = 540^\circ\text{C}$ is similar to that of layers annealed at 600°C . These overlayers produced LEED spots that are nearly as sharp as those produced by the substrates. Although annealing reduced the background intensity, it did not cause the domains to grow. Analysis of the data obtained from the as-grown overlayer ($T_s = 540^\circ\text{C}$) shows that the overlayer is free of monatomic steps within experimental error. Figure 1 shows a plot of these angular widths of the Ge (01) beam plotted as $\Delta S_{||}/[\Delta S_{||}]_{BZ}$ versus S_{\perp} . The slope corresponds to a mosaic spread of $\pm 0.12^\circ$. The curve intersects the ordinate axis at $[\Delta S_{||}/[\Delta S_{||}]]_{BZ} = 0.024$, corresponding to a domain size of $\sim 210 \pm 40\text{\AA}$. This represents the largest domain size for Ge that we have been able to obtain in these experiments.

There may be two mechanisms that influence the observed structural order of the epitaxial overlayers. The first is basically a kinetic limitation operative during the growth process at low temperatures (i.e. $T_s = 450^\circ\text{C}$) that causes the overlayer to be highly stepped or rough.

An explanation for the finite-size effects that are observed following the annealing treatments is that they are a result of substrate defects that were induced during the cleavage process. It is well known that nucleation of overlayers occurs at defects on a substrate surface, such as cleavage steps.⁽¹¹⁾ Dislocations may be initiated in the growing film at the edges of the slip planes. The annealing process allows these dislocations to climb to the surface of the film, making a true mosaic on the surface. The estimated terrace width if the broadening is due to slip planes, 280\AA , is nearly identical to the largest domain size that we have observed in the Ge overlayers.

In summary, we have demonstrated that it is possible to extract quantitative information on structural defects even for (1×1) overlayers using LEED. For epitaxial growth of Ge on GaAs(110) under the present experimental conditions, the overlayers appear to have a higher concentration of extended defects than the substrates on which they are grown. At low growth temperatures, this may be due to a mechanism that inhibits layer-by-layer growth, causing the surface to be highly stepped. For annealed layers, dislocations grown into the film may propagate to the surface and cause the Ge layer to be polycrystalline but still oriented. The symmetry of the patterns differs from that observed by Mönch and Gant.⁽⁵⁾ It is possible that the appearance of superlattices is related to growth mode.

Slip planes in the substrate may also serve as barriers to adatom diffusion during the initial stages of epitaxy. For low coverages (less than a few monolayers), the film will thus consist of islands that are the same size, or smaller than, the terraces between slip planes. We are at present investigating this by growing films that are a few monolayers thick and analyzing the corresponding LEED patterns.

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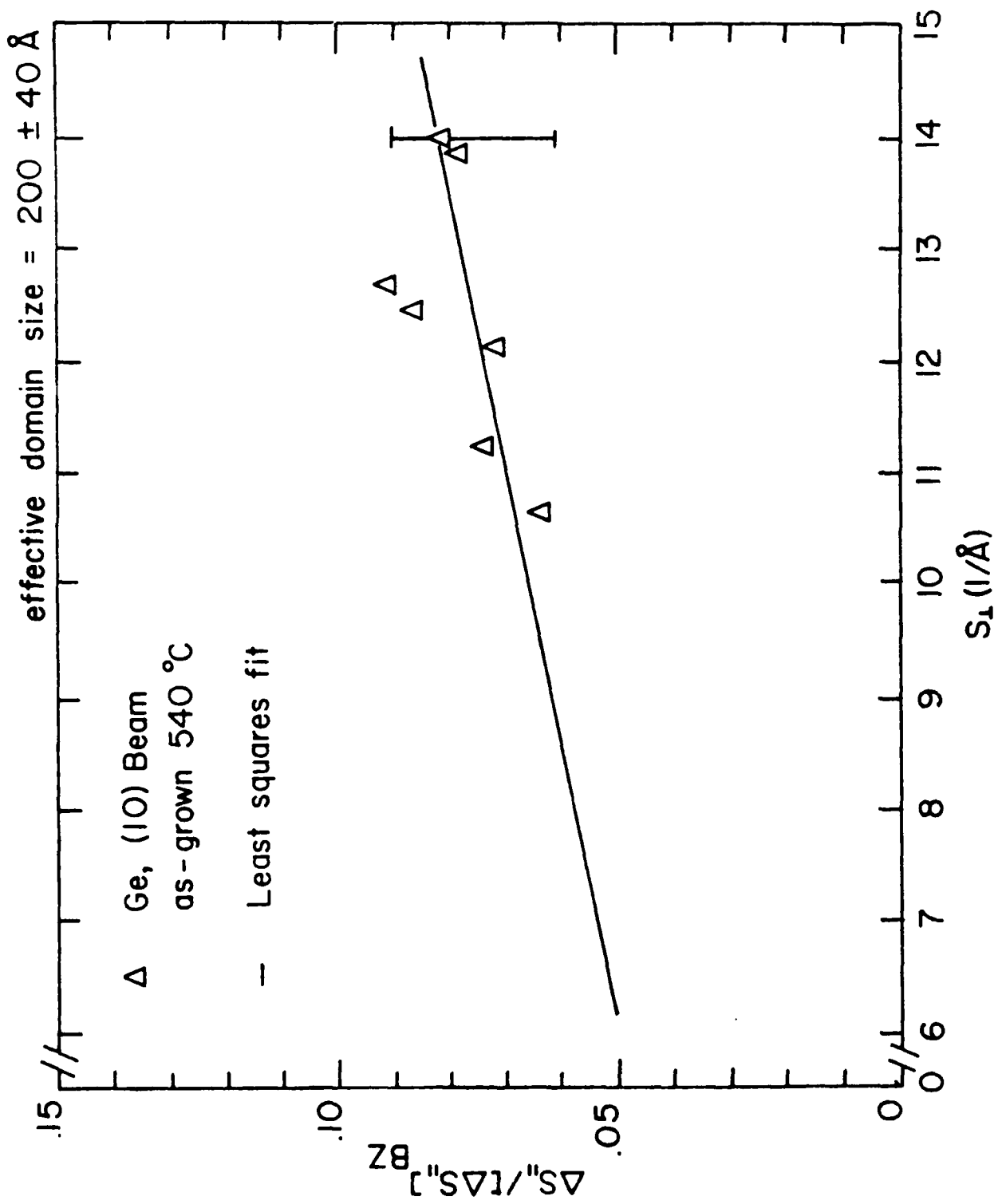
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Figure Captions

Figure 1. Angular width of the (01) beam for the Ge overlayer grown at $T_s = 540^\circ\text{C}$, as a function of S_L . The slope corresponds to an out-of-plane misorientation of $\pm 0.12^\circ$. The intercept of the line with $S_L = 0$ gives the finite size of the overlayer domains, in this case $\sim 210\text{\AA}$. $\Delta S_{||}/[\Delta S_{||}]_{\text{BZ}}$ is the FWHM of the diffraction spot expressed as a fraction of the Brillouin zone width in reciprocal space.



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